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MASTER

COMPARISON OF EXPERIMENTALLY DETERMINED SPENT-FUEL COMPOSITIONS WITH ORIGEN2 CALCULATIONS

Allen G. Croff

Chemical Technology Division
Oak Ridge National Laboratory*
Oak Ridge, Tennessee

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Prior to the development of the ORIGEN2 code,[1,2] it was recognized that verification of the calculated data was needed. Unfortunately, there were no well-characterized, experimentally based spent fuel compositions for modern LWRs that could be used to validate the fuel depletion calculations since the existing studies included no measurements which would allow independent determination of the burnups of the relatively small samples. Since that time, however, well-characterized experimental work has been completed and documented,[3] allowing a comparison with calculated results.

The specific experimental measurements of interest here involve the determination of parameters related to the actinide and fission product composition of samples from five elements taken from fuel assemblies discharged from the Turkey Point Unit 3 PWR. Two fuel assemblies (D01 and D04) were obtained for the purposes of nondestructive and destructive assay. These assemblies were initially fueled with 448 kg of UO_2 enriched to 2.556 wt % ^{235}U and then irradiated for 851 full-power days. Five elements were then removed, and assay samples were taken from each element near the core midplane. The relevant parameters measured were $^{148}Nd/^{238}U$, $^{239}Pu/^{238}U$, and the isotopic compositions of U, Pu, Kr, and Xe.

Fuel depletion calculations were performed using the updated ORIGEN2 PWR model.[4] The burnup of the fuel was determined by adjusting the ORIGEN2 fuel burnup to match the experimentally determined $^{148}Nd/^{238}U$ ratio for each fuel element. The resulting burnup was then used to calculate the other experimentally determined parameters listed above.

The sample burnups and a comparison of the experimental and calculated actinide parameters are given in Table 1. As is evident, the agreement between ORIGEN2 and the experimental results is very good, with the average error for five samples being <4% for most parameters. The $^{235}U/U$ ratio is high because the calculation is sensitive to errors in differences as the two values involved approach zero. If instead the average error is based on the depletion of ^{235}U, the result is an error of $-2.3 \pm 1.6\%$. The other relatively large error is the -7.6% for the $^{242}Pu/Pu$ ratio, although the absolute differences between the ORIGEN2 and experimental values are small. The reason for this relatively large error cannot be determined until experimental data on the transplutonic nuclide composition of the fuel become available.

The comparisons of the isotopic compositions of krypton and xenon are given in Table 2. The values for all five samples have been averaged due to the reduced number of significant digits available from the experimental work. As is evident, the agreement is excellent in all instances save the $^{85}Kr/Kr$ ratio. The fact that only the radioactive nuclide in Table 2 has a significant deviation indicates that a decay correction may be needed. A possible explanation for this is that the noble gases are released to the plenum (where the sample was taken) only during the initial stages of irradiation and that these gases then decay for the rest of the irradiation. This hypothesis is supported by experimental results[3] which show that only about 0.2% of the noble gases produced in the fuel are found in the plenum gas.

Based on this comparison, it appears that the ORIGEN2 computer code is capable of accurately calculating the composition of irradiated fuel from a modern PWR. However, well-characterized experimental measurements should continue to be obtained for validation purposes because the calculated values of many nuclides, particularly the minor actinides, still have significant uncertainties.

Table 1. Comparison of Experimental (EXP) and ORIGEN2 Results for the Actinides

Measured parameter (atom %)	Sample designation[a]										Average error[c] (%) ± standard deviation
	D01-G10-4		D01-G9-15		D04-G9-9		D04-G10-7		D01-H9-7		
	EXP[b]	ORIGEN2	EXP	ORIGEN2	EXP	ORIGEN2	EXP	ORIGEN2	EXP	ORIGEN2	
$^{239}Pu/^{238}U$	0.507	0.527	0.507	0.528	0.518	0.529	0.502	0.530	0.517	0.530	3.6 ± 1.4
$^{235}U/U$	0.599	0.662	0.619	0.655	0.582	0.637	0.598	0.635	0.590	0.627	7.7 ± 2.2[d]
$^{236}U/U$	0.342	0.334	0.342	0.334	0.332	0.337	0.342	0.337	0.334	0.338	-0.7 ± 1.9
$^{238}Pu/Pu$	1.545	1.456	1.561	1.472	1.535	1.514	1.570	1.517	1.592	1.537	-4.0 ± 1.8
$^{239}Pu/Pu$	54.757	56.000	55.107	55.850	54.654	55.480	54.574	55.450	54.806	55.280	1.5 ± 0.5
$^{240}Pu/Pu$	25.846	25.150	25.701	25.180	25.553	25.280	25.851	25.290	25.411	25.330	-1.7 ± 1.0
$^{241}Pu/Pu$	11.988	12.120	11.984	12.170	12.329	12.250	12.113	12.260	12.177	12.300	0.9 ± 0.9
$^{242}Pu/Pu$	5.864	5.269	5.647	5.325	5.929	5.470	5.892	5.481	6.014	5.549	-7.6 ± 1.6
Burnup, MWd/MTHM[e]		29,625		29,829		30,353		30,402		30,645	

[a] Assembly-rod-axial location.

[b] Data from ref. 3.

[c] (ORIGEN2 - EXP) x 100/EXP.

[d] If ^{235}U depletion is used as a basis, the average error becomes -2.3 ± 1.6%.

[e] Burnup that results in equal experimental and ORIGEN2 $^{148}Nd/^{238}U$ ratios.

Table 2. Comparison of Experimental and ORIGEN2 Results for Noble Gases

Measured parameter (atom %)	Experimental average over 5 fuel elements[a,b]	ORIGEN2 average over 5 fuel elements[a]
$^{82}Kr/Kr$		0.3
$^{83}Kr/Kr$	12.0	11.6
$^{84}Kr/Kr$	32.4	31.6
$^{85}Kr/Kr$	4.2	5.5
$^{86}Kr/Kr$	51.4	51.0
$^{130}Xe/Xe$		0.3
$^{131}Xe/Xe$	8.2	8.4
$^{132}Xe/Xe$	20.8	20.9
$^{134}Xe/Xe$	28.0	27.6
$^{136}Xe/Xe$	43.0	42.8

[a] Elements are the same as those in Table 1.

[b] Data from ref. 3.

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